Statistical and Low Temperature Physics (PHYS393)

0. Background
1. Basic statistics

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0. Background

What this course is about.

The first part of this course is Statistical Mechanics. Starting from Schrödinger's equations for electrons and atoms, we learn how to calculate the macroscopic properties in thermodynamics, such as entropy and heat capacity.

The second part is about experimental methods at low temperatures. We learn how statistical mechanics can be used to understand the behaviour of matter at very low temperatures, and to develop the cooling techniques needed to reach these temperatures.

1. Statistical Mechanics - A Survival Guide,
   A. M. Glazer and J. S. Wark
   Oxford University Press, 2001
   Chapters 1 - 9
   (available as ebook in Liverpool University library).

2. Matter and Methods at Low Temperatures,
   Frank Pobell
   Springer; 2nd edition,2002
   Chapter 1, and
   sections 2.1-2.3.3, 3.1, 4.1-4.2, 5.1-5.2.4, 6.1, 7.1-7.2,
   9.1-9.4, 10.1-10.2
   (available as ebook in Liverpool University library)

3. Lecture notes from previous lecturers, available on VITAL.

Physics

1. Thermodynamics (PHYS253)

   This is covers most of the basic ideas. It would be helpful if you could look through your lecture notes again.

2. Quantum and Atomic Physics (PHYS255)

   You would need the following: particle in a box, simple harmonic oscillator, Zeeman effect, fermions and bosons.

3. The mole concept

   `http://en.wikipedia.org/wiki/Mole_(unit)`

Maths

1. Logarithms, permutations, differentiations, integration

   http://en.wikipedia.org/wiki/Logarithm
   http://en.wikipedia.org/wiki/Combination
   http://en.wikipedia.org/wiki/Logarithm
   http://en.wikipedia.org/wiki/Derivative

   http://en.wikipedia.org/wiki/Antiderivative

2. Statistics

   http://en.wikipedia.org/wiki/Expected_value
   http://en.wikipedia.org/wiki/Variance

   http://en.wikipedia.org/wiki/Binomial_distribution

3. Lagrange multipliers

   http://en.wikipedia.org/wiki/Lagrange_multipliers

$$\int_0^\infty x^{2n+1} e^{-a^2x^2} dx = \frac{n!}{2a^{2n+2}}$$

$$\int_{-\infty}^\infty x^{2n} e^{-a^2x^2} dx = \frac{(2n)!\pi^{1/2}}{n!(2a)^{2n}a}$$

$$\int_0^\infty \frac{x^{1/2}}{e^x - 1} dx = 2.32$$

$$\int_0^\infty \frac{x^{3/2}}{e^x - 1} dx = 1.78$$

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$$

Physical constants

Electron rest mass	m_e	$9.109 \times 10{-}31$ kg
Proton rest mass	m_p	1.6726×10^{-27} kg
Atomic mass unit	u	1.6605×10^{-27} kg
Electronic charge	e	1.6022×10^{-19} C
Speed of light in free space	c	2.9979×10^{8} m s^{-1}
Planck's constant	h	6.626×10^{-34} J s
	$h/2\pi = \hbar$	1.0546×10^{-34} J s
Boltzmann's constant	k_B	1.3807×10^{-23} J K^{-1}
Gas constant	R	8.314 J mol^{-1} K^{-1}
Avogadro constant	N_A	6.022×10^{23} mol^{-1}
Standard molar volume		22.414×10^{-3} m^3 mol^{-1}
Bohr magneton	μ_{B}	9.274×10^{-24} J T^{-1}
Nuclear magneton	μ_{n}	5.051×10^{-27} J T^{-1}
Stefan's constant	σ	5.671×10^{-8} W m^{-2} K^{-4}
Gravitational constant	G	6.673×10^{-11} N m^2 kg^{-2}
Proton magnetic moment	μ_{p}	$2.7928\mu_{\mathrm{N}}$
Neutron magnetic moment	μ_{p}	$-1.9130\mu_{\mathrm{N}}$
Acceleration due to gravity	g	9.807 m s^{-2}
Permeability of free space	μ_0	$4\pi \times 10^{-7}$ H m^{-1}
Permittivity of free space	ϵ_0	8.854×10^{-12} F m^{-1}

Part 1: Statistical Mechanics

Part 2: Low Temperature Cooling Techniques

Part 1: Statistical Mechanics

1. Basic statistics

Aim

To understand the basic statistical methods required.

Objectives

1. To write down the outcomes of tossing a coin.
2. To explain the microstate and the macrostate.
3. To predict the most probable macrostate in coin tossing.
4. To explain the terms expectation, variance and standard deviation.
5. To use the binomial distribution in coin tossing.
6. To describe the most probable macrostate for large number of tosses.

1.1 Tossing a coin

We often use the familiar coin tossing to develop the techniques. There is a rather broad analogy with the quantum mechanics:

1. Head or tail – 2 energy levels
2. Many coins – many atoms
3. number of heads - energy, or temperature

Define the notations:

H = head
T = tail

Suppose we toss a coin 4 times. The possible outcomes are:

4 heads (4H), or HHHH

3 heads 1 tail (3H1T). This could be in different orders:
HHHT, HHTH, HTHH or THHH.

2 heads 2 tails (2H2T)

and so on.

There are a few ways to describe the outcome.

If we say 3H1T, we know there is only 1 tail, but we don't know the order of tail.

If we say HTHH, then we know it is the second toss that is tail.

We shall use the following 2 ways:

1. Macrostate.

   Some, but not all details are specified, such as 3H1T. It is the set of all outcomes that have the specified features.

2. Microstate.

   This is a full description, such as HTHH. This tells us the exact outcome.

When we toss a coin 4 times, we can define a macrostate by the number of H. Then there are 5 macrostates:

x	Macrostate	Microstates
0	4T	TTTT
1	1H3T	TTTH, TTHT, THTT, HTTT
2	2H2T	HHTT, HTHT, THHT, THTH, TTHH, HTTH
3	3H1T	HHHT, HHTH, HTHH, THHH
4	4H	HHHH

The most probable macrostate is the one with the most microstates. That would be 2H2T, or $x = 2$.

Let

$N =$ no. of times to flip the coin
$\Omega =$ no. of times to get n heads

Using combinations ($^N C_n$), we find

$$\Omega = \frac{N!}{n!(N-n)!} \tag{1}$$

We can use this to find the number of microstates. We flip the coin 4 times, so $N = 4$. For the macrostate 2H2T, $n = 2$.

The above formula gives the number of microstate as $\Omega = 4!/(2!2!) = 6$, which is what we got on the previous page.

1.2 Probability, mean and standard deviation

We are interested in the properties macroscopic objects with very large number of atoms.

The total energy of the atoms would determine the temperature of an object.

At room condition, the object temperature stays constant, even though individual atoms would change energies through vibration.

Imagine tossing a coin a large number of times. Would the total number of heads stay relative constant?

We can find out using the binomial distribution.

Suppose a coin is tossed 2 times. The possible outcomes are:
TT
HT
TH
HH

Let x be the number of heads. Let n be the total number of outcomes.

Let $P(x)$ be probability of getting x heads. This is given by $P(x) = x/n$.

$P(0) = 1/4$
$P(1) = 2/4$
$P(2) = 1/4$

Suppose we toss the coin n times and record the number of H. Suppose we repeat this many times.

We would get a sample of data for x, e.g. $\{$2, 0, 1, 3, 2, 2, 3, 0, ... $\}$

In statistics, we are often interested in two numbers - the mean and the standard deviation.

The mean is the simple average.

The standard deviation tells us how much the numbers in the data deviate from the mean.

If we know the probaility distribution $P(x)$, we can also calculate the mean and standard deviation without actually tossing the coin.

The mean is given by

$$\mu = \sum xP(x).$$

The standard deviation is the root mean square of $x - \mu$. So it is essentially a kind of average of how much x deviates from μ.

It is given by

$$\sigma = \sqrt{\sum(x-\mu)^2 P(x)}.$$

More explanation can be found in:

http://en.wikipedia.org/wiki/Expected_value
http://en.wikipedia.org/wiki/Standard_deviation

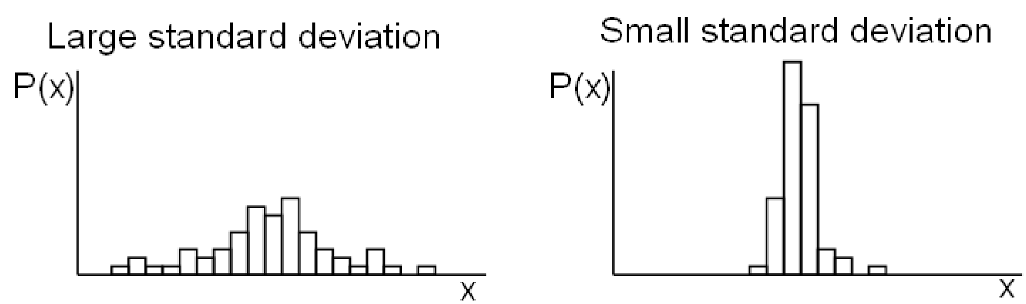
When the standard deviation is small

The standard deviation is relevant to the idea of macrostates that we want to develop.

We are particularly interested in what it means if the standard deviation becomes very small.

Recall that the standard deviation is a measure of the average deviation of x from the mean.

So if the standard deviation is small, it means that most of the data is very close to the mean value.



If we look at a histogram of the data, it would look more sharply peaked.

1.3 Coin tossing and temperature

A hot cup of tea contains an extremely large number of molecules of water rapidly exchanging energy with one another, and with the surrounding cup and air. At any one time, the energy of a particular molecule could quite random.

Yet, over the period of a few minutes, the temperature of the tea would remain fairly constant.

The temperature is a measure of the total energy of the molecules.

Suppose we toss a number of coins. Each time we toss, theoutcome of a particular coin would be random.

Suppose the coin is the molecule. Suppose further that T is the ground state and H the excited state of 2 energy levels.

The total number of H would then be the total energy, or temperature. We would of course expect this total to be quite different each time we toss.

But what if we have an extremely large number of coins? Is it possible then that the total number would not change very much?

It turns out that we can calculate this deviation quite easily using the binomial distribution.

Let p be probability of getting a Head, and q the probaility of getting a Tail.

If we have a fair coin, then $p = q = 1/2$.

Suppose we toss a coin N times.

The probaility of getting x heads is given by the binomial distribution:

$$P(x) =^N C_n p^n q^{N-n}.$$

For an explanation of this formula, see:

http://en.wikipedia.org/wiki/Binomial_distribution

When we toss a coin N times, suppose that we get x heads.

When we toss N times again, we are likely to get a different x.

The mean value of x is given by a sum over x, weighted by the probabilities:

$$\mu = \sum_{x=0}^{N} xP(x) = Np.$$

The standard deviation is given by:

$$\sigma = \sqrt{\sum_{x=0}^{N} (x-\mu)^2 P(x)} = \sqrt{Npq}.$$

Both formulae can be derived by substituting the binomial distribution $P(x) =^N C_n p^n q^{N-n}$.

Lets get some idea of how σ changes a N is increased. For a fair coin $p = q = 1/2$.

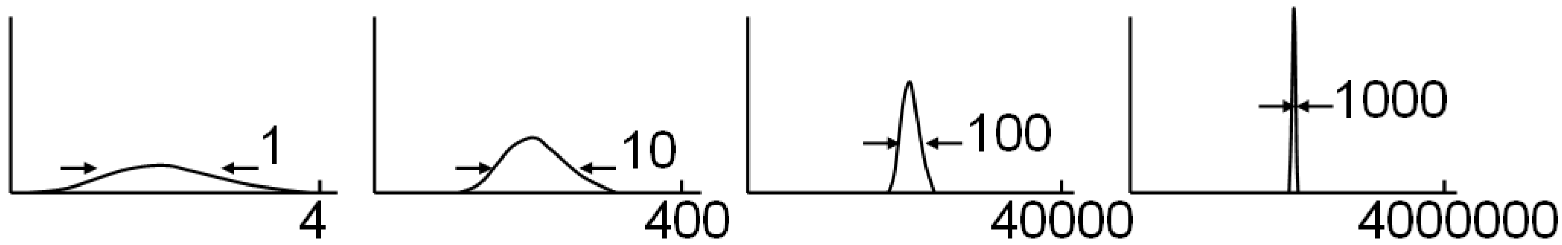
N	$\sigma(=\sqrt{Npq})$
4	1
400	10
40000	100
4000000	1000

It looks like the number of heads changes more from one toss to the next, as the number of coins is increased.

But if we plot the distribution on a graph:

we would find that it gets more sharply peaked!

The reason is because, on the graph, we are looking at the standard deviation relative to the total number of coins N.



So, although 10 is large than 1, 10/400 would be smaller than 1/4.

This way of looking at it reminds us that to determine whether the change of a quantity is large, we need to have something meaningful to compare with.

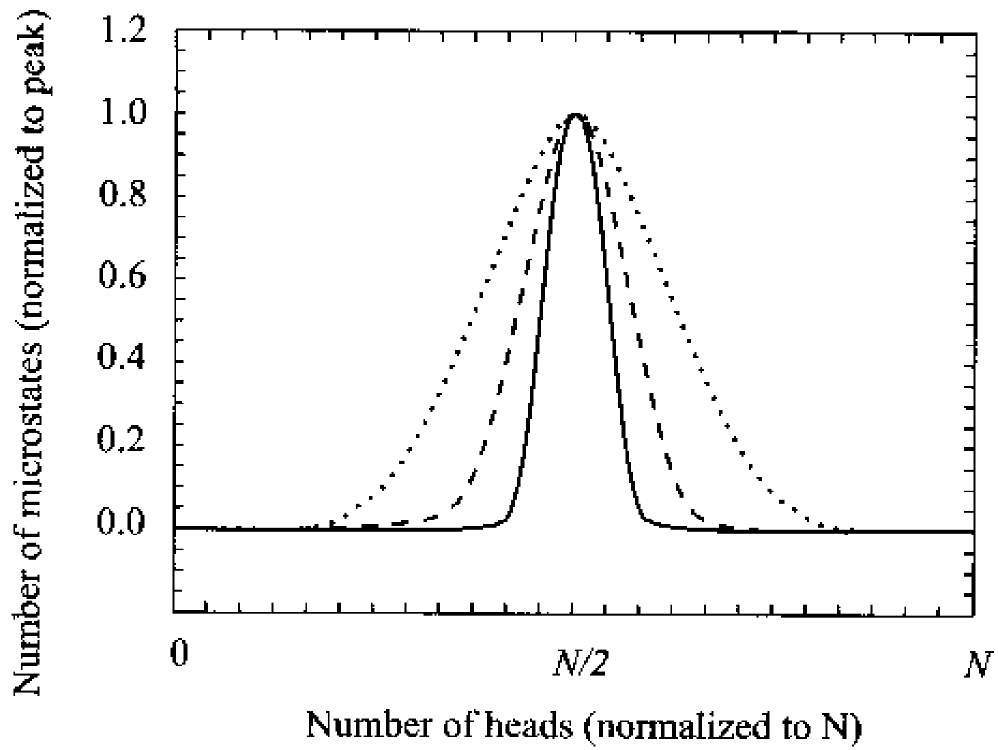
For example, when we say the temperature of a cup of tea does not change much, we are really comparing it with the temperature of the tea itself, which could be at 70 deg Celsius, or 343 K.

In the case of the coins, we should therefore be comparing the standard deviation with the total number of coins N.

x is the actual number of heads in one microstate.

The average of deviation of this number from the mean, as a fraction of N, is $\sigma/N = \sqrt{pq/N}$.

When N is very large, this fraction approaches zero.



The dotted curve is the smallest N, the solid curve the largest N. Notice that the peak gets narrower for large N.

If N is as big as the number of atoms in a real material, the peak becomes extremely narrow.

Then $x = N/2$ becomes almost the only macrostate.

Very broadly, we may draw the following analogy:

1. H is the higher energy state, T is the lower one.

2. One toss of a coin is one atom.

3. The number of H is the temperature.

In a real material at room temperature, each atom could take on energy random, through colliding with other atoms.

Because the number of atoms is huge, when we measure the temperature with a thermometer, we hardly see any fluctuation - even though the energy of each atom is changing all the time.

1. A coin may represent a particle with two energy levels.
2. The macrostate could be specified by the number of heads, and the microstate by the actual ordering.
3. The most probable macrostate in coin tossing is $x = N/2$.
4. The binomial distribution can be used to calculate the mean and standard deviation in coin tossing.
5. For large number of tosses, it is very unlikely to have macrostates different from $x = N/2$.

Exercise 1

Suppose a biased coin is tossed 2 times. The probability distribution for 0, 1 and 2 heads are given by 0.36, 0.48 and 0.16, respectively. Find the mean and standard deviation of the number of heads.

Answer

Let x be the number of heads. The distribution given is

x	$P(x)$
0	0.36
1	0.48
2	0.16

The mean is $\mu = \sum xP(x) = 0 \times 0.36 + 1 \times 0.48 + 2 \times 0.16 = 0.8$.

(Out of 2 tosses, we only get 0.8 heads on average. Obviously, this coin is biased towards the tail.)

x	$x - \mu$	$(x-\mu)^2$
0	-0.8	0.64
1	0.2	0.04
2	1.2	1.44

The standard deviation is

$$\sigma = \sqrt{\sum (x-\mu)^2 P(x)}$$

$$= \sqrt{0.64 \times 0.36 + 0.04 \times 0.48 + 1.44 \times 0.16} = 0.48.$$